

09/ 832 786
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NEWS 10 DEC 17 COMPUAB reloaded; updating to resume; current-awareness
alerts (SDIs) affected
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NEWS 13 DEC 17 THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS 14 DEC 30 EPFULL: New patent full text database to be available on STN
NEWS 15 DEC 30 CAPLUS - PATENT COVERAGE EXPANDED
NEWS 16 JAN 03 No connect-hour charges in EPFULL during January and
February 2005

NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT
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AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
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=> FIL MEDLINE CAPLUS
COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'MEDLINE' ENTERED AT 12:24:06 ON 11 JAN 2005

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=> s docking and (rms or "root mean square")

L1 180 DOCKING AND (RMS OR "ROOT MEAN SQUARE")

=> s l1 and "common core"

L2 0 L1 AND "COMMON CORE"

=> s l1 and cluster

L3 5 L1 AND CLUSTER

=> d l3 1-5

L3 ANSWER 1 OF 5 MEDLINE on STN

AN 2003258922 MEDLINE

DN PubMed ID: 12784373

TI Successful discrimination of protein interactions.

AU Camacho Carlos J; Gatchell David W

CS Department of Biomedical Engineering, Boston University, Boston,
Massachusetts 02215, USA.. ccamacho@bu.edu

NC GM61867-01 (NIGMS)

SO Proteins, (2003 Jul 1) 52 (1) 92-7.

Journal code: 8700181. ISSN: 1097-0134.

CY United States

DT (EVALUATION STUDIES)

Journal; Article; (JOURNAL ARTICLE)

LA English

FS Priority Journals

EM 200308

ED Entered STN: 20030605

Last Updated on STN: 20030813

Entered Medline: 20030812

L3 ANSWER 2 OF 5 MEDLINE on STN

AN 97031795 MEDLINE

DN PubMed ID: 8877701

TI Distributed automated **docking** of flexible ligands to proteins:
parallel applications of AutoDock 2.4.

AU Morris G M; Goodsell D S; Huey R; Olson A J

CS Department of Molecular Biology, MB-5, Scripps Research Institute, La
Jolla, CA 92037, USA.

NC GM48870-01 (NIGMS)

RR08065 (NCRR)

SO Journal of computer-aided molecular design, (1996 Aug) 10 (4) 293-304.

Journal code: 8710425. ISSN: 0920-654X.

CY Netherlands

DT Journal; Article; (JOURNAL ARTICLE)

LA English

FS Priority Journals; AIDS

EM 199703

ED Entered STN: 19970407

Last Updated on STN: 19980206

Entered Medline: 19970325

L3 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:472214 CAPLUS

DN 139:209536

TI Successful discrimination of protein interactions
 AU Camacho, Carlos J.; Gatchell, David W.
 CS Department of Biomedical Engineering, Boston University, Boston, MA, USA
 SO Proteins: Structure, Function, and Genetics (2003), 52(1), 92-97
 CODEN: PSFGEY; ISSN: 0887-3585
 PB Wiley-Liss, Inc.
 DT Journal
 LA English
 RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2002:158328 CAPLUS
 DN 136:194220
 TI Prioritization of combinatorial library screening
 IN Diller, David J.; Merz, Kenneth M.
 PA USA
 SO U.S. Pat. Appl. Publ., 25 pp., Cont.-in-part of U.S. Ser. No. 595,096.
 CODEN: USXXCO
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002025535	A1	20020228	US 2001-832786	20010411
	WO 2001097098	A2	20011220	WO 2001-US19318	20010615
	WO 2001097098	A3	20030828		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 2003228624	A1	20031211	US 2002-320752	20021216
PRAI	US 2000-595096	A2	20000615		
	US 2001-832786	A	20010411		
	WO 2001-US19318	A1	20010615		

L3 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1998:793720 CAPLUS
 DN 130:148165
 TI ELECT + +: faster conformational search method for **docking** flexible molecules using molecular similarity
 AU Makino, Shingo; Kuntz, Irwin D.
 CS Department of Pharmaceutical Chemistry, School of Pharmacy, University of California, San Francisco, CA, 94143-0446, USA
 SO Journal of Computational Chemistry (1998), 19(16), 1834-1852
 CODEN: JCCHDD; ISSN: 0192-8651
 PB John Wiley & Sons, Inc.
 DT Journal
 LA English
 RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> FIL PATENTS

FILE 'ENCOMPPAT' ACCESS NOT AUTHORIZED
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SINCE FILE ENTRY TOTAL SESSION

FULL ESTIMATED COST

28.72

28.93

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 CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE 'WPIFV' ENTERED AT 12:38:14 ON 11 JAN 2005
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=> s docking and "root mean square" and "common core"
 17 FILES SEARCHED...
 34 FILES SEARCHED...
 L4 12 DOCKING AND "ROOT MEAN SQUARE" AND "COMMON CORE"

=> s l4 not py>2001
 6 FILES SEARCHED...
 22 FILES SEARCHED...
 '2001' NOT A VALID FIELD CODE
 34 FILES SEARCHED...
 L5 3 L4 NOT PY>2001

=> d 15 1-3

L5 ANSWER 1 OF 3 PCTFULL COPYRIGHT 2005 Univentio on STN
AN 2001097098 PCTFULL ED 20020826
TIEN MOLECULAR DOCKING METHODS FOR ASSESSING COMPLEMENTARITY OF
COMBINATORIAL LIBRARIES TO BIOTARGETS
TIFR PROCEDES D'AMARRAGE MOLECULAIRE PERMETTANT D'ESTIMER LA COMPLEMENTARITE
DE BIBLIOTHEQUES COMBINATOIRES POUR DES BIOCIABLES
IN DILLER, David, J.;
MERZ, Kenneth M., Jr.
PA PHARMACOPEIA, INC.;
DILLER, David, J.;
MERZ, Kenneth M., Jr.
DT Patent
PI WO 2001097098 A2 20011220
DS W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CR CU CZ
DE DK DM DZ EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP
KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX
MZ NO NZ PL PT RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA
UG US UZ VN YU ZA ZW GH GM KE LS MW MZ SD SL SZ TZ UG ZW
AM AZ BY KG KZ MD RU TJ TM AT BE CH CY DE DK ES FI FR GB
GR IE IT LU MC NL PT SE TR BF BJ CF CG CI CM GA GN GW ML
MR NE SN TD TG
AI WO 2001-US19318 A 20010615
PRAI US 2000-09/595,096 20000615
US 2001-09/832,786 20010411
ICM G06F017-50

L5 ANSWER 2 OF 3 PCTFULL COPYRIGHT 2005 Univentio on STN
AN 1997027559 PCTFULL ED 20020514
TIEN METHOD OF CREATING AND SEARCHING A MOLECULAR VIRTUAL LIBRARY USING
VALIDATED MOLECULAR STRUCTURE DESCRIPTORS
TIFR PROCEDE POUR CREER UNE BIBLIOTHEQUE MOLECULAIRE VIRTUELLE ET PROCEDE
POUR Y FAIRE DES RECHERCHES, EN UTILISANT DES DESCRIPTEURS VALIDES DE
STRUCTURE MOLECULAIRE
IN PATTERSON, David, E.;
CRAMER, Richard, D.;
CLARK, Robert, D.;
FERGUSON, Allan, M.
PA PATTERSON, David, E.;
CRAMER, Richard, D.;
CLARK, Robert, D.;
FERGUSON, Allan, M.
LA English
DT Patent
PI WO 9727559 A1 19970731
DS W: AU CA CN CZ HU IL JP KR NO PL US AT BE CH DE DK ES FI FR
GB GR IE IT LU MC NL PT SE
AI WO 1997-US1491 A 19970127
PRAI US 1996-8/592,132 19960126
US 1996-8/657,147 19960603
ICM G06F019-00

L5 ANSWER 3 OF 3 USPATFULL on STN
AN 2001:80395 USPATFULL
TI Further method of creating and rapidly searching a virtual library of
potential molecules using validated molecular structural descriptors
IN Cramer, Richard D., O'Fallon, MO, United States
Patterson, David E., St. Louis, MO, United States
PA Tripos, Inc., St. Louis, MO, United States (U.S. corporation)
PI US 6240374 B1 20010529
AI US 1997-903217 19970720 (8)
RLI Continuation-in-part of Ser. No. US 1996-657147, filed on 3 Jun 1996,

now abandoned Continuation-in-part of Ser. No. US 1996-592132, filed on
26 Jan 1996

DT Utility

FS Granted

LN.CNT 5284

INCL INCLM: 703/011.000

INCLS: 703/012.000; 435/007.100; 435/DIG.051

NCL NCLM: 703/011.000

NCLS: 435/007.100; 435/DIG.051; 703/012.000

IC [7]

ICM: G06F001-00

ICS: G06F003-00; G06F007-00; G06F007-06

EXF 702/27; 702/19; 702/22; 435/7.1; 435/DIG.51; 364/496; 703/11; 703/12

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